Progress in the Optical Measurement and Modeling of Multilayer Thin Film Solar Cell Structures*

R.W. Collins, [1] G.M. Ferreira, [1] A. Ferlauto, [1] C. Chen, [1] C.R. Wronski, [1] X. Deng, [2] and G. Ganguly [3]

(1) Materials Research Laboratory and Center for Thin Film Devices, The Pennsylvania State University, University Park, PA 16802; (2) Department of Physics and Astronomy, University of Toledo, Toledo, OH 43606; (3) BP Solar, 3601 LaGrange Parkway, Toano, VA 23168.

ABSTRACT

In this research effort, we focus on methods for enhancing optical collection and reducing optical losses in so-called "specular" a-Si:H-based p-i-n solar cell structures for building-integrated photovoltaics applications. The optical simulations performed in this study have been made possible by the development of an extensive optical property database for the solar cell component layers. Using this database in the simulations, we have identified the beneficial effects of a microscopic roughness layer at the SnO_2/p interface. This roughness layer reduces the interface dielectric discontinuity, and hence acts as an anti-reflector. We have also identified the detrimental effects of a chemically-intermixed region at the ZnO/Ag interface of the retroreflecting structure. This intermixed region acts as a parasitic absorber. Non-idealities at both interfaces can have significant impacts on the generated currents, yet have not been considered in detail in previous studies. The general approaches established in this research effort can also be applied in other thin film photovoltaics technologies.

1. Introduction

In simulations of the optical quantum efficiency (QE) of a-Si:H-based solar cells, the complicated light-trapping effects of macroscopic roughness in so-called "textured" structures have been widely considered [1]. In contrast, the simpler effects of microscopic roughness in "specular" structures have been widely ignored. In fact for building-integrated photovoltaics applications, the macroscopic roughness of textured structures is undesirable due to their hazy appearance. As a result, the optical simulation of specular solar cell structures is an important research activity with the goal being to identify methods for enhancing the optical collection without texture and for reducing optical losses.

Microscopic roughness is defined as surface/interface modulations with in-plane correlation lengths at least an order of magnitude smaller than the center wavelength λ_c of the incident light beam. (λ_c~500 nm for solar cells.) The optical effect of microscopic interface roughness can be simulated by inserting a layer at the interface whose thickness scales with the rms roughness and whose optical properties are determined from an effective medium theory assuming a composite of the overlying and underlying materials [2]. In contrast, macroscopic roughness is defined as modulations with in-plane correlation lengths within an order of magnitude of λ_c. The optical effect of macroscopic roughness at an interface is a reduction in the specularly reflected and transmitted electric field amplitudes in accordance with scalar diffraction theory [3]. This reduction is offset by non-specularly scattered field components in the reflected and transmitted waves that appear as "haze".

In this study, we explore the effects on the simulated optical QE due to microscopic roughness and chemically intermixed layers at interfaces of transparent conducting oxide layers in the specular a-Si:H solar cell structure. Here, the nature of the interface layers has been deduced independently from ex situ, in situ, and real time spectroscopic ellipsometry (SE) of photovoltaic structures, and the effects of these layers on the QE of the solar cell are determined. This approach is in contrast to the usual one for optical modeling in which inputs of the simulation routines are chosen to yield outputs in qualitative agreement with experimental QE curves. The latter approach is not reliable unless the simulation routines include the complete optical physics of the problem.

2. Modeling Results and Discussion

Next, we describe applications of the optical property database established previously [4] to assess the impact of interface non-idealities on optical collection in single-junction a-Si:H-based solar cells having a specular structure. In the multilayer optical analysis used here, incoherent multiple reflections within the glass substrate and coherent reflections within all other layers are assumed in order to compute the optical characteristics of the solar cells. These characteristics include the absorbance for each layer and the reflectance for the entire structure. Because the Ag back-reflector incorporated into the cell structure is opaque, the spectral transmittance is zero. Thus, photon flux that is not absorbed in the a-Si:H i-layer will be absorbed in the other layers and lost, or reflected from the entire structure and lost. The basic solar cell structure consists of glass/SnO_2/p-i-n/ZnO/Ag, where we use our database for the optical properties of each of the component layers [4].

Figure 1 (upper panel) shows the difference between the spectral absorbances in the i-layer (fractions of incident irradiance absorbed) for a solar cell structure with a 45 nm microscopic roughness layer at the SnO_2/p interface and for an ideal structure with no interface roughness. In the former solar cell structure, microscopic roughness layers are also incorporated at the successive interfaces of the device (e.g., p/i, i/n, n/ZnO) in proportion to that at the SnO_2/p interface as has been measured in previous real-time SE studies [3]. The ZnO/Ag interface in both structures of Fig. 1, however, is assumed to be ideal. The lower panel of Fig. 1 shows the corresponding difference in the spectral reflectances for the two structures (rough–ideal). The most important effect of microscopic roughness at the solar cell interfaces is an increase in the total photon flux collected by the i-layer. The maximum gain is observed near 550 nm. The potential increase in short-circuit current ΔJ_{SC} for the solar cell (computed by integrating the product of the optical quantum efficiency and the AM1.5 spectral photon flux over the range from 270 to 900 nm) as a result of these microscopic roughness layers is ~0.7 mA/cm^2.

The optical gains in Fig. 1 associated with the microscopic roughness layers are attributed to the suppression of refractive index discontinuities. In fact, the strongest effect occurs at the SnO_2/p interface, where the discontinuity is the
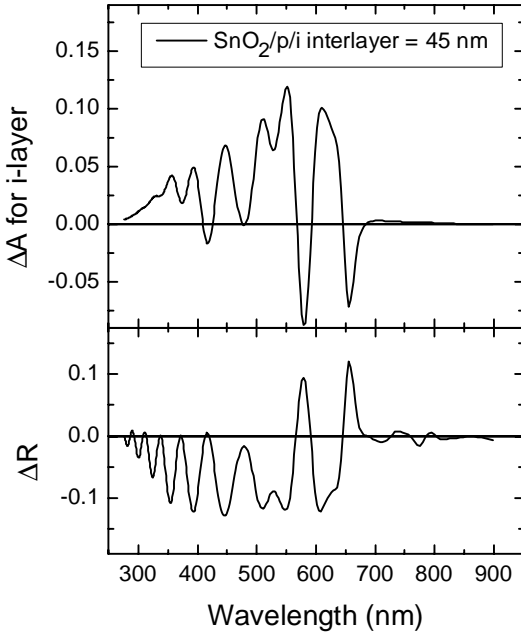
Fig. 1 Predicted increase in the i-layer absorbance spectrum (upper panel) for an a-Si:H p-i-n solar cell obtained by assuming a 45 nm microscopic roughness layer at the SnO_2/p-layer interface, over that for an "ideal" device without interface roughness. The lower panel shows the difference (rough − ideal) in the solar cell reflectance spectra.
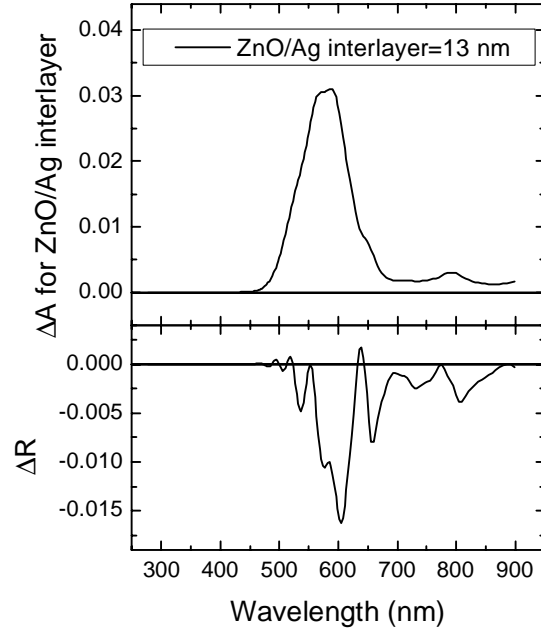

Fig. 2 Predicted increase in parasitic absorbance (upper panel) of the ZnO/Ag interface in the a-Si:H p-i-n solar cell obtained upon introduction of a 13 nm ZnO/Ag interlayer (21/79 vol.% ZnO/Ag). The lower panel shows the difference (interlayer − ideal) in the solar cell reflectance spectra.

largest and the roughness layer is the thickest. Thus, the microscopic roughness layer acts as an anti-reflecting layer for this interface; irradiance that would otherwise be reflected from the SnO_2/p interface in an ideal structure passes into the i-layer where it can be absorbed.

Figure 2 (upper panel) shows the increase in back-reflector absorbance that results when a 13 nm ZnO/Ag interface layer is incorporated into the solar cell structure having 45 nm roughness at the SnO_2/p interface. The interface layer in this case is attributed not only to microscopic roughness but also to atomic-scale intermixing and interface reactions when Ag is sputtered on ZnO (or vice versa in an n-i-p solar cell). The optical properties of the interface layer are simulated as a 0.21/0.79 mixture of ZnO/Ag, applying the Bruggeman effective medium theory. The result of Fig. 2 shows a significant parasitic absorbance loss due to the interface layer in the spectral region from 500 to 700 nm. With decreasing wavelength below 500 nm, the decrease in absorbance loss is attributed to the fact that almost all incident irradiance is absorbed by the overlying structure, whereas the decrease with increasing wavelength above 700 nm appears to be an effect of the optical properties of the interface layer. The latter effect is expected to be strongly dependent on the chemical and microstructural nature of the interface layer. The lower panel of Fig. 2 provides the corresponding difference in reflectance (interlayer − ideal). The potential gain ΔJ_{SC} that would occur if all the parasitic absorbance losses in the ZnO/Ag interface region could be converted to useful current is ~0.55 mA/cm^2 in this case.

3. Summary

In previous research, we have developed analytical expressions that describe the optical properties of the components of a-Si:H-based solar cells. Such expressions will assist in the future in modeling the optical performance of the solar cells and will allow the user to tailor the optical properties based on physical inputs. These inputs include the optical gaps of the i-layers, the free carrier concentration of the transparent conductors, and the grain size of the metallic back-reflectors. Our approach is quite general and can also be applied to other thin film solar cell technologies, as well. In this recent study, we have demonstrated the capabilities of such modeling by assessing the impact of SnO_2/p-layer microscopic roughness on carrier collection in the a-Si:H i-layer of a single-junction p-i-n solar cell, and also the effect of an imperfect ZnO/Ag interface layer on the absorbance of the back reflector structure. In these two examples, we demonstrate how the nature of the interfaces in the a-Si:H solar cell can have a significant impact on the performance of the device, and emphasize that a reliable set of optical properties is required to assess this impact.

4. References

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